CHM129
Gibbs Free Energy

1. Use ΔG°_{Rxn} to determine whether the process is spontaneous. Calculate the value of the equilibrium constant, K.

$$2\ NO_{(g)} + O_{2\ (g)} \rightarrow 2\ NO_{2\ (g)}$$

	ΔH°_f (kJ/mol)	S° (J/mol.K)
NO	+90.29	+210.65
O_2	0	+205.0
NO_2	+32.2	+239.9

$\Delta H^\circ_{Rx} = \Sigma n \Delta H_f^\circ \text{ prod} - \Sigma n \Delta H_f^\circ \text{ react.}$

$= (2 \text{ mol} \times 32.2 \text{ kJ/mol}) - [(2 \text{ mol} \times 90.29 \text{ kJ/mol}) + (1 \text{ mol} \times 0 \text{ kJ/mol})]$

$\Delta H^\circ_{Rx} = -116.2 \text{ kJ}$

$\Delta S^\circ_{Rx} = \Sigma n S^\circ \text{ prod} - \Sigma n S^\circ \text{ react.}$

$= (2 \text{ mol} \times 239.9 \text{ J/mol·K}) - [(2 \text{ mol} \times 210.65 \text{ J/mol·K}) + (1 \text{ mol} \times 205.0 \text{ J/mol·K})]$

$\Delta S^\circ_{Rx} = -146.5 \text{ J/K} = -0.1465 \text{ kJ/K}$

$\Delta G^\circ_{Rx} = \Delta H^\circ - T\Delta S^\circ$

$= -116.2 \text{ kJ} - (298 \text{ K})(-0.1465 \text{ kJ/K})$

$\Delta G^\circ_{Rx} = -72.5 \text{ kJ}$

$\Delta G < 0$ Rx is spontaneous

$K = e^{-\Delta G^\circ/RT}$

$\dfrac{\Delta G^\circ}{RT} = \dfrac{(-72.5 \text{ kJ})}{(8.314\times10^{-3} \frac{\text{kJ}}{\text{mol·K}})(298 \text{ K})}$

$= -29.3$

$K = e^{-(-29.3)} = 5\times10^{12}$

2. (a) Calculate the standard free energy ($\Delta G°$) and the equilibrium constant (K) at 298K for the following reaction:

$$H_{2(g)} + Br_{2(g)} \leftrightarrow 2\ HBr_{(g)}$$

Is the process spontaneous as written?

HBr: $\Delta G°_f$ = -53.22 kJ/mol   **H_2:** $\Delta G°_f$ = 0 kJ/mol   **Br_2:** $\Delta G°_f$ = 0 kJ/mol

(b) If you have a reaction mixture with initial concentrations $[H_2]$=0.200M and $[Br_2]$=0.200M, what are the equilibrium concentrations of H_2, Br_2, and HBr?

(a) $\Delta G^o_{Rx} = \Sigma n\,\Delta G^o_f\ \text{prod} - \Sigma n\,\Delta G^o_f\ \text{react}$

$= (2\ \text{mol} \times -53.22\ \text{kJ/mol}) - [(1\ \text{mol} \times 0\ \text{kJ/mol}) + (1\ \text{mol} \times 0\ \text{kJ/mol})]$

$\Delta G^o_{Rx} = -106.4\ \text{kJ}$

$\Delta G < 0 \Rightarrow$ Rx is spontaneous.

$K = e^{-\Delta G/RT}$

$\frac{\Delta G}{RT} = \frac{-106.4}{(8.314\times10^{-3})(298)} = -42.9$

$K = e^{-(-42.9)} = \underline{4\times10^{18}}$

$K \gg 1$ Products (forward Rx) Favored

(b) $K = \frac{[HBr]^2}{[H_2][Br_2]} = 4\times10^{18}$

	$[H_2]$	$[Br_2]$	$[HBr]$
I	0.200	0.200	0
C	$-x$	$-x$	$+2x$
E	$0.200-x$	$0.200-x$	$2x$

$\frac{(2x)^2}{(0.200-x)(0.200-x)} = 4\times10^{18}$

$\frac{2x}{0.200-x} = \sqrt{4\times10^{18}}$

$2x = \sqrt{4\times10^{18}}\,(0.200-x)$

$x = 0.2M$

$[H_2] = [Br_2] = 0.200M - 0.2M = \underline{0\ M}$

$[HBr] = 2(0.2M) = \underline{0.4\ M}$